The conserved-order-parameter Ising model

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1 Introduction

The conserved-order-parameter Ising model (COP Ising model) is a model mathematically similar to the normal Ising model, but it simulates very different systems. While the normal Ising model is a good description of a ferromagnet, the COP Ising model studies lattice gases.

1.1 The Lattice Gas

A lattice gas is a simple model of a gas, where a large number of particles (atoms or molecules) can only move on the vertices of a lattice. The lattice is not really there, it is just a discretisation of space to simplify the calculations. Although this discretisation makes the model less realistic, it can still give a good insight into the general behaviour of real gases.
There are a few variations, that can be build into the model of lattice gases:

- The lattice itself can take different shapes (square, hexagon, simple cubic, face-centred cubic, ...).
- More than one type of particles.
- Different particle interactions.
- The particles can have inertia.

2 The Model

The simplest model for a lattice gas has particles with no inertia, who move on the lattice by a random walk representing thermal excitation with a temperature T. If we have a lattice with N sites and a fraction ρ ("particle density") is occupied by particles, then these particles satisfy following rules:

1. The particle density ρ is constant.
2. A lattice site can be occupied by at most one particle.
3. If two particles occupy nearest-neighbour sites on the lattice, they feel an attraction with a fixed energy ϵ.

Rules 2 and 3 are approximations for the forces between particles in real gases. In terms of the Lennard-Jones-Potential the short-ranged repulsion is rule 2 and the long-ranged attraction is rule 3. However in this approximation there is no short- and long-ranged, because both forces work on the same distance of the nearest-neighbour. Nonetheless the described model is useful, because it possesses a phase transition between a homogeneous gas phase and a solid/vapour coexistence phase. The phase of the lattice gas depends on the temperature T and the density ρ:

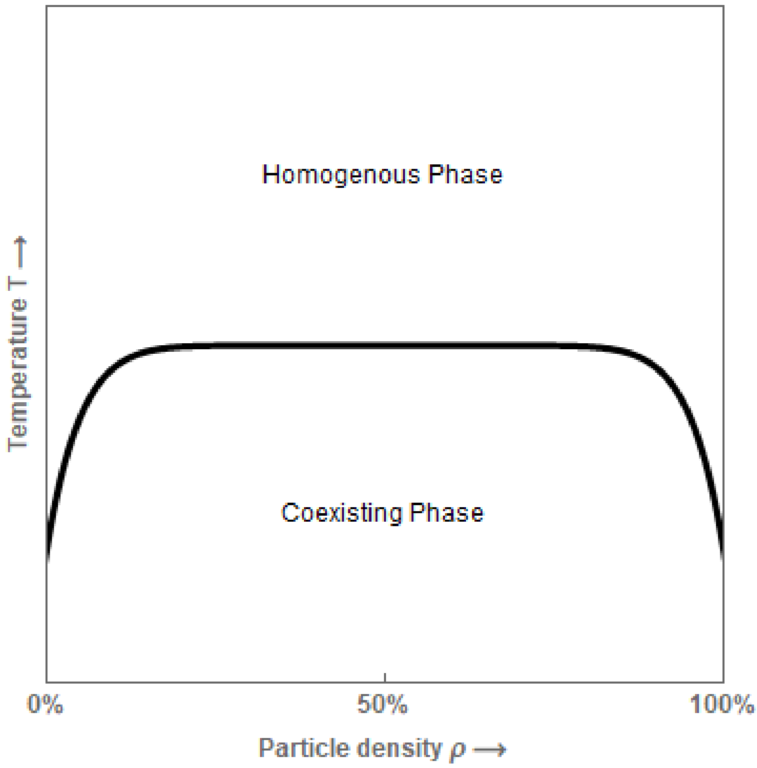

Figure 1: Example for a phase diagram of a two-dimensional lattice gas with a square lattice.

In the vicinity of the phase transition some properties of the model become independent of the exact interactions between the particles and the model becomes capable of making quantitative predictions about real gases.

To study our model of the lattice gas we have to derive the Hamiltonian H of the system. First we define the variables σ_i, one for each lattice site (i=1,2,...,N). σ_i holds the information whether the lattice site i is occupied or not:

$$\sigma_i = \begin{cases} 0 & \text{if site is free} \\ 1 & \text{if site is occupied} \end{cases} .$$

With this notation rule 2 is obeyed, because a lattice site can either be occupied or not. To ensure that rule 1 is obeyed, we require that the number of particles is a constant:

$$\sum_i \sigma_i = \rho N \quad . \tag{1}$$

Rule 3 defines the Hamiltonian H of our model. If two particles occupy two nearest-neighbour sites, then they contribute an energy $-\epsilon$ to the system:

$$H = -\epsilon \sum_{\langle i,j \rangle} \sigma_i \sigma_j \quad , \tag{2}$$

where $\langle i, j \rangle$ are the lattice sites which are nearest-neighbours.

2.1 Equivalence to the normal Ising Model

The simplest model for a lattice gas is equivalent to the ferromagnet in the normal Ising model. To show this we define a new variable for each lattice site i:

$$s_i = 2\sigma_i - 1 \quad . \tag{3}$$

It is easy to see that s_i can either by -1 for a free site or $+1$ for a occupied site, which shows that s_i is the same as the spins in the normal Ising model.
If we solve (3) for σ_i and substitute it into (2), we get:

$$\begin{aligned} H &= -\frac{1}{4}\epsilon \sum_{\langle i,j \rangle} (s_i + 1)(s_j + 1) \\ &= -\frac{1}{4}\epsilon \left(\sum_{\langle i,j \rangle} s_i s_j + \sum_{\langle i,j \rangle} s_i + \sum_{\langle i,j \rangle} s_j + \sum_{\langle i,j \rangle} 1 \right) \\ &= -\frac{1}{4}\epsilon \sum_{\langle i,j \rangle} - \frac{1}{2}\epsilon z \sum_i s_i - \frac{1}{2}\epsilon z N \end{aligned} \tag{4}$$

With the lattice coordination number z, which is equal to the number of nearest-neighbours each lattice site has (e.g. for a square lattice: z=4).
If we substitute (3) into (1), we get an expression for the sum over s_i:

$$\sum_i s_i = N(2\rho - 1) \quad . \tag{5}$$

Substituting this into (4), we get:

$$H = -\frac{1}{4}\epsilon \sum_{\langle i,j \rangle} s_i s_j - \epsilon z N \rho \quad . \tag{6}$$

The second term of (6) is a constant and if we define $\epsilon/4 = J$, we get:

$$H = -J \sum_{\langle i,j \rangle} s_i s_j + costant \quad , \tag{7}$$

which (except for the constant) is identical to the Hamiltonian of the normal Ising model with no magnetic field.
Although the Hamiltonians are identical, we still have to consider the first rule, expressed in (1) or (5):

$$\begin{aligned} \sum_i s_i &= N(2\rho - 1) \\ \Rightarrow \qquad M &= N(2\rho - 1) \quad , \end{aligned} \tag{8}$$

where M is the magnetization.
The right site of (8) is a constant. Thus the magnetization M is also constant and therefore we call this model the conserved-order-parameter Ising model.

3 Phase Transition

The phase transition of the simplest lattice gas can be explained through the equivalence to the normal Ising model.
Form the normal Ising model, we know that there exists a critical temperature T_c, where the average of the magnetization M is zero above T_c and non-zero below. Rearranging (8) for ρ we get:

$$\begin{aligned} \rho &= \frac{1}{2}\left(1 + \frac{M}{N}\right) \\ \Rightarrow \rho &= \frac{1}{2}(1 + m) \quad , \end{aligned} \tag{9}$$

where m is the magnetization per spin.
Below the critical temperature T_c, the magnetization per spin m has two equilibrium values with the same magnitude but opposite signs. Thus also the density ρ has two preferred values:

$$\rho_+ = \frac{1}{2}(1 + |m|) \quad \wedge \quad \rho_- = \frac{1}{2}(1 - |m|) \tag{10}$$

The equilibrium value of the magnetization per spin m depends on the Temperature T. If the temperature T is high, the magnetization per spin m is small and above T_c, m is zero.

For the COP Ising model the density ρ is a constant. If we chose a value for ρ, which satisfies:

$$\rho_- \leq \rho \leq \rho_+$$

for a temperature below T_c, we observe a phase separation into domains of the preferred values. Meaning that the density ρ is not homogeneous and that there are regions in the lattice gas with a high density ρ_+ and others with a low density ρ_-. Above the critical temperature T_c there is equilibrium value of m and the range of ρ shrinks to zero: $\rho_- = \rho_+ = \rho$. The lattice gas is in the homogeneous phase.